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A finite elements model including surface contribution in micromagnetic simulation

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ABSTRACT

This work presents micromagnetic simulations of the behavior of ferromagnetic particles, carried out by use of the finite element method, taking into account, in a special way, the peculiarity of the surface. Results including the role of the surface in the various mechanisms of magnetization reversal, like the coherent rotation, the vortex creation and the nucleation/expansion of magnetic domains, as dictated by the magnitude of the particles, are presented and commented upon.

1. Introduction

It is widely accepted and proven that surface effects play a crucial role in the magnetic behavior of materials [1]. Broken bonds, vacancies, reduced dimensionality and stresses lead to misalignment between the surface and main volume magnetic moments, and that because of surface structure defects, which affect intrinsic properties like the magnetization, the direction and strength of the anisotropy and the exchange length. Surface contributions are clearly evident in structures where the surface to volume ratio is quite large, as nanoparticles and thin films [2,3]. This does not mean that surface contribution can be omitted in large particles. As already mentioned by Givord et al. [4] about the physics of coercivity, the magnetization reversal is constituted by a series of local processes, of which the first, the nucleation of a reverse magnetization domain, takes place within a local (surface) defect.

Modeling of the surface effects can be carried out by atomistic models, as the Monte Carlo [5] method, and also by continuous micromagnetic models using either the finite difference [6] or the finite element techniques [7]. But simulations of this kind are limited at the nanoscale, firstly because of the great importance of the surface in this region and secondly due to intensive increment of computational cost with respect to the size.

From the theoretical point of view, Brown's micromagnetic model [8] states that the surface requires a special treatment and needs to be described by an additional contribution in the free energy. But in Brown's equation, first of all, the surface exchange torque will emerge from the volume exchange – energy integral in the variational procedure and not as an independent term of the free energy, thus the surface exchange has only normal to the surface component and not tangential. Secondly, the surface anisotropy is introduced as an external torque with normal to surface component in order to balance the exchange torque. But the latter is not the general case, because the anisotropy axis can be randomly directed or pointing to a specific crystallographic direction [9].

In this work micromagnetic simulations are presented by means of Finite Element Method (FEM) based on a model in which surface contribution is approximated by an additional and different set of partial differential equations (PDE), which includes tangential variations. The latter are to be solved only for the surface nodes, thus highly reducing computational cost, and enabling simulations of large particles.

2. Simulation model

In this model the evolution of the magnetization vector is not described by the trivial approach of the Landau–Lifshitz–Gilbert (LLG) equation. In the continuum scheme, the derivation of the PDE is based on a Lagrangian approach, assuming that the rotation of the magnetization vector $\vec{M}$ in a elementary volume can be described by that of a rigid current loop [10]. The resulting PDE has

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the form

$$\left[\frac{\partial^2\vec{M}}{\partial t^2}-\left(\frac{\vec{M}}{M_s^2}\cdot\frac{\partial^2\vec{M}}{\partial t^2}\right)\vec{M}\right]+\frac{1}{\tau}\frac{\partial\vec{M}}{\partial t}=\frac{\mu_o v}{I}\left(\vec{M}\times\vec{\mathcal{H}}\right)\times\vec{M} \quad (1)$$

where M_s is the saturation magnetization, v and I is the volume and the moment of inertia associated with the current loop respectively and τ is the relaxation time of the system, assuming a homogenous and isotropic Rayleigh type dissipation.

$\vec{\mathcal{H}}$ is a local effective field that can be defined by the variational derivative of the free micromagnetic energy. The main contributions to the micromagnetic energy arise from exchange, magnetocrystalline, magnetostatic and Zeeman energies. In this context, assuming a uniaxial anisotropy

$$\vec{\mathcal{H}}=\ell^2\nabla^2\vec{M}+\kappa^2\left(\hat{u}\cdot\vec{M}\right)\hat{u}+\vec{H}_d+\vec{H}+\vec{H}_{th} \quad (2)$$

where $\ell=\sqrt{2A/\left(\mu_o M_s^2\right)}$ is the exchange length with A the exchange stiffness, $\kappa=\sqrt{2K_1/\left(\mu_o M_s^2\right)}$ is the hardness parameter with K_1 the first order anisotropy constant and $\hat{u}$ the direction of the easy axis. In the absence of conducting media, the demagnetizing field, $\vec{H}_d$, can be calculated from the gradient of a magnetic scalar potential φ, which obeys the Poisson equation $\nabla^2\varphi=-\nabla\cdot\vec{M}$. Finally, $\vec{H}$ is the external applied field and $\vec{H}_{th}$ is an artificial thermal field, added to overcome the unstable equilibrium states, where no torque acts on the magnetization. This field is thought as a Gaussian random process in space, obeying $\vec{H}_{th}\left(\vec{r}\right)\cdot\vec{H}_{th}\left(\vec{r}'\right)=H_{th}^2\delta\left(\vec{r}-\vec{r}'\right)$. The smaller the amplitude H_{th} becomes, a greater delay in the response of the system appears. On the other hand, at high values of H_{th} artificial thermal effects affect the results. In order to establish the optimal value for H_{th}, we examine the behavior of a spherical particle of radius R under conditions of coherent rotation reversal ($\ell/R=1$). The anisotropy field was set to $0.2M_s$ and the external field was applied parallel to the easy axis and varied very slowly from M_s to $-M_s$. By varying the H_{th}, an estimation of the coercive field H_c is made, which according to the Stoner–Wohlfarth theory is equal to the anisotropy field. For H_{th} lower than $10^{-3}M_s$ the coercive field agrees with theory and, under these considerations, the was set to $10^{-4}M_s$ for all simulations.

In the case of high damping limit, the acceleration term (the term inside brackets in Eq. (1) can be omitted, and the above PDE takes the form

$$C\frac{\partial\vec{M}}{\partial t}=\left(\vec{M}\times\vec{\mathcal{H}}\right)\times\vec{M} \quad (3)$$

with $C=I/(\mu_o\tau v)\left[A^2m^{-2}s\right]$, which describes the evolution of the magnetization vector in the case of slowly varying external fields with respect to the time constant C/M_s^2.

Using this approach, the three PDE for magnetization components and the one for magnetic scalar potential are solved simultaneously through the FEM. A weak form is derived by means of the weighted residual approach supported with the Galerkin method.

The integral equation for each of the magnetization components, $M_r(r=x,y,z)$, has the form

$$\int_V w_r\left[C\frac{\partial M_r}{\partial t}-\mathcal{H}_r+\left(\vec{\mathcal{H}}\cdot\vec{M}\right)M_r\right]dv=0, \quad (4)$$

where w_r is the corresponding set of weighted functions, $\mathcal{H}_r$ is the r-component of the effective field and V is the volume of the magnetic domain. Splitting the effective field in two parts, one arising from exchange ($\ell^2\nabla^2\vec{M}$) and one from all the other mechanisms ($\vec{\mathcal{H}}'$), i.e., $\vec{\mathcal{H}}=\vec{\mathcal{H}}'+\ell^2\nabla^2\vec{M}$, the integral equation takes the form

$$\int_V w_r\left[C\frac{\partial M_r}{\partial t}-\mathcal{H}_r'+\left(\vec{\mathcal{H}}'\cdot\vec{M}\right)M_r-\ell^2\nabla^2M_r+\ell^2\left(\vec{M}\cdot\nabla^2\vec{M}\right)M_r\right]dv=0. \quad (5)$$

The first exchange term in the above equation can be replaced under vector identity with

$$w_r\ell^2\nabla^2M_r=\nabla\cdot\left(w_r\ell^2\nabla M_r\right)-\nabla\left(w_r\ell^2\right)\cdot\nabla M_r. \quad (6)$$

Due to the preservation of the magnetization norm, the equation

$$\vec{M}\cdot\frac{\partial\vec{M}}{\partial q}=0\{q=x,y,z\} \quad (7)$$

holds. Differentiating once with respect to the three spatial variables and summing the produce equations results in

$$\left(\frac{\partial\vec{M}}{\partial x}\right)^2+\left(\frac{\partial\vec{M}}{\partial y}\right)^2+\left(\frac{\partial\vec{M}}{\partial z}\right)^2=-\vec{M}\cdot\nabla^2\vec{M}. \quad (8)$$

Thus the second exchange term in the Eq. (5) is written as

$$w_r\ell^2\left(\vec{M}\cdot\nabla^2\vec{M}\right)M_r=-w_r\ell^2M_r\sum\nolimits_{p,q}\left(\frac{\partial M_p}{\partial q}\right)^2\quad\{p,q=x,y,z\}. \quad (9)$$

Replacing and applying the divergence theorem, the final form of the integral equation is

$$\int_V\left[w_rC\frac{\partial M_r}{\partial t}-w_r\mathcal{H}_r'+w_r\left(\vec{\mathcal{H}}'\cdot\vec{M}-\ell^2\sum_{p,q}\left(\frac{\partial M_p}{\partial q}\right)^2\right)M_r+\nabla\left(\ell^2w_r\right)\cdot\nabla M_r\right]dv$$
$$-\int_S w_r\ell^2\frac{\partial M_r}{\partial n}ds=0, \quad (10)$$

where S is the magnetic domain surface to the non magnetic environment and n is the unit normal vector to this surface.

In the general case all the magnetic parameters $(M_s,A,K_1,\hat{u})$ vary in space, but in the case of a homogeneous single crystal particle, variations can only take place near the surface. In order to simulate the surface contribution, the particle must be separated in two magnetic domains, one for the main volume and one for the surface layer. However, this method becomes very expensive, from computational aspects, when the volume to surface ratio becomes very large, due to very dense discretization needed. One approach to the problem is to consider a surface layer with very small thickness (for example equal to the unit cell), where the magnetization vector is not varied along the thickness coordinate. This can be accepted, considering that the unit cell size is generally smaller than the domain wall width (Table 1). Then the volume integral equation for each magnetization component becomes a surface integral equation

$$\int_{S_{hl}}\left[aw_rC_I\frac{\partial M_r}{\partial t}-aw_r\mathcal{H}_{Ir}'+aw_r\left(\vec{\mathcal{H}}_I'\cdot\vec{M}-\ell_I^2\sum_{p,q_T}\left(\frac{\partial M_p}{\partial q_T}\right)^2\right)M_r\right.$$
$$\left.+a\ell_I^2(\nabla_Tw_r\cdot\nabla_TM_r)-w_r\ell^2\frac{\partial M_r}{\partial n}ds=0\right. \quad (11)$$

Table 1
Critical lengths for some magnetic materials [16].

Magnetic material	a (Max unit cell dimension) [nm]	$\ell\left(\sqrt{2A/\mu_oM_s^2}\right)$ [nm]	$\delta(2\ell/\kappa)$ [nm]	a/ℓ	a/δ
$Ni_{80}Fe_{20}$	0.352	4.81	1273	0.07	0.0003
Fe	0.287	3.39	41	0.08	0.007
Co	0.407	4.81	15	0.08	0.027
$Nd_2Fe_{14}B$	1.218	2.69	2	0.45	0.49
$SmCo_5$	0.499	5.09	2	0.10	0.30
Fe_3O_4	0.840	6.93	46	0.12	0.02
$BaFe_{12}O_{19}$	2.319	8.20	9	0.28	0.27